Low Energy of Activation Lithium-Ion Conducting Channel

IUSRT-4 **22 Sep 2010**

Dr. Lawrence Scanlon
Thermal & Electrochemical Branch
Propulsion Directorate
Air Force Research Laboratory

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED
SEP 2010	**N/A**	**-**

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Low Energy of Activation Lithium-Ion Conducting Channel	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Thermal & Electrochemical Branch Propulsion Directorate Air Force Research Laboratory**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release, distribution unlimited

13. SUPPLEMENTARY NOTES
See also ADA560467. Indo-US Science and Technology Round Table Meeting (4th Annual) - Power Energy and Cognitive Science Held in Bangalore, India on September 21-23, 2010. U.S. Government or Federal Purpose Rights License

14. ABSTRACT

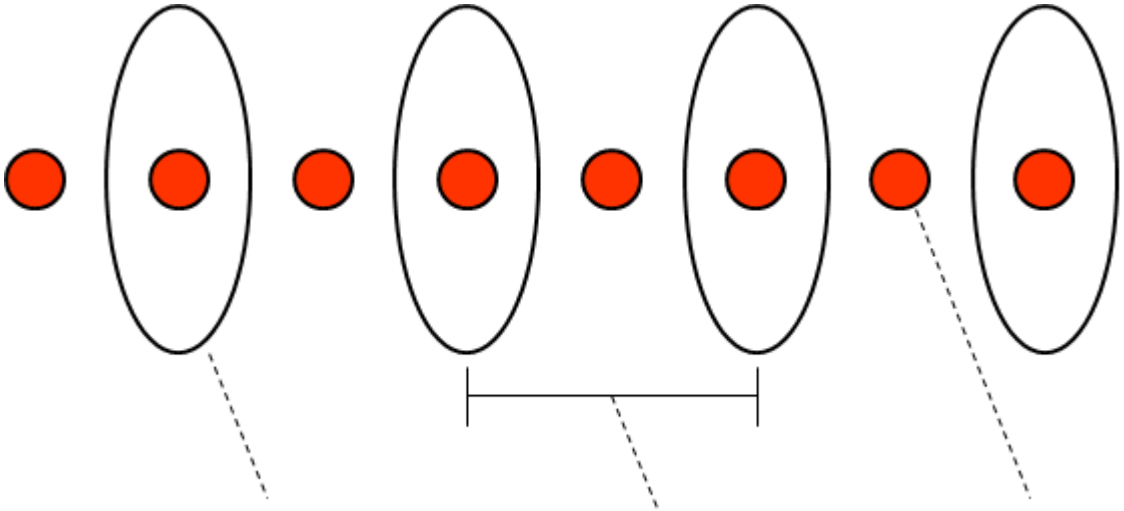
15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			
unclassified	**unclassified**	**unclassified**	**SAR**	**15**	

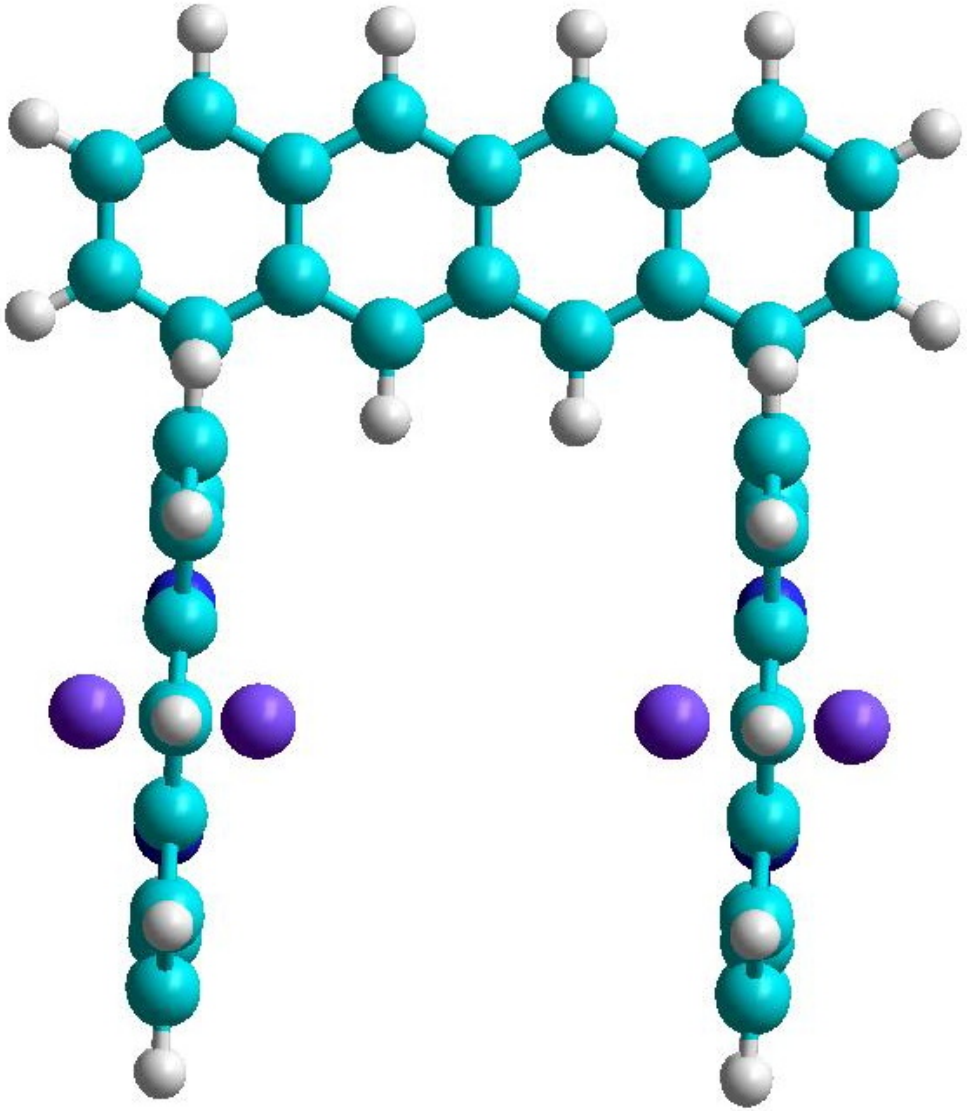
Outline

- **Lithium Ion Conducting Channel**
- **Negative Electrostatic Potential field**
  - Electron Delocalization
- **Low Energy of Activation**
  - Single Crystals
  - Thin Film
- **Conclusion**

Conceptualized Lithium-Ion Conducting Channel



Channel Concept Based on Tetracene Bridging Unit with Dilithium Porphyrins Attached



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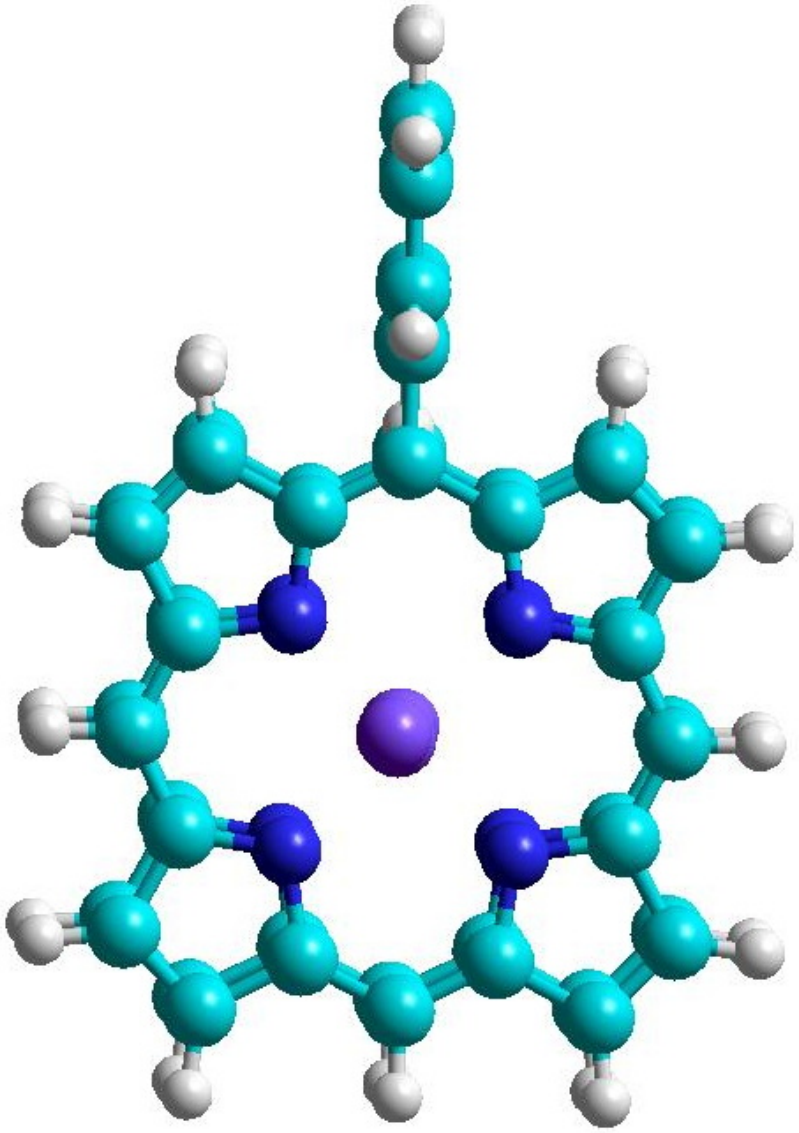
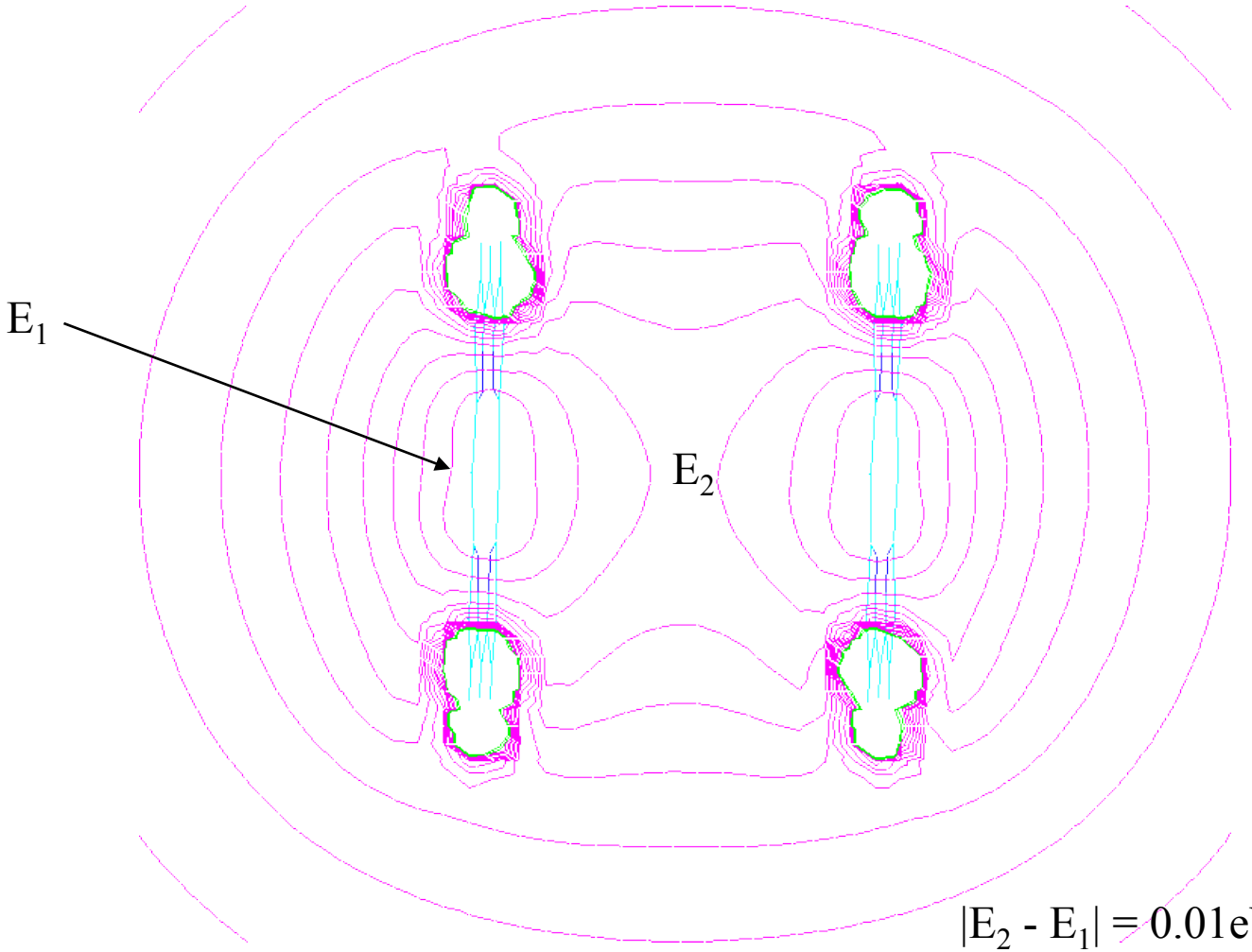
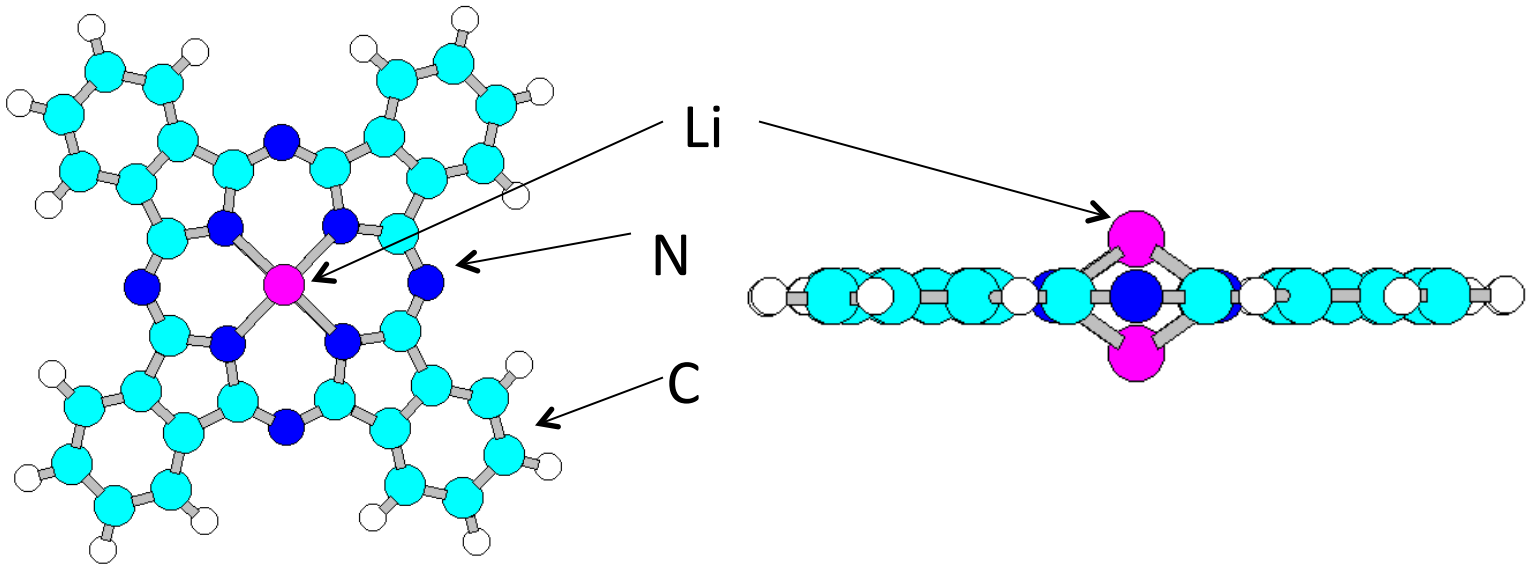


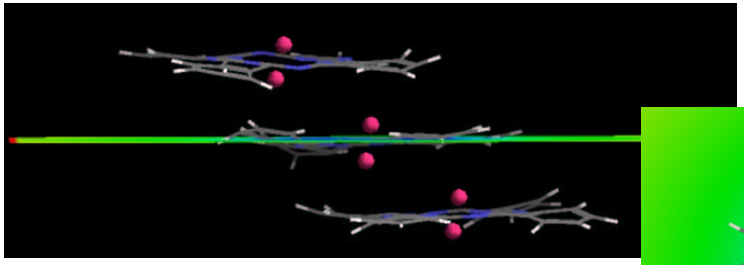
Negative Electrostatic Potential Contours for Two Porphyrin Dianions Separated by 7 Å. (E_2, E_1 - Electrostatic Potential)

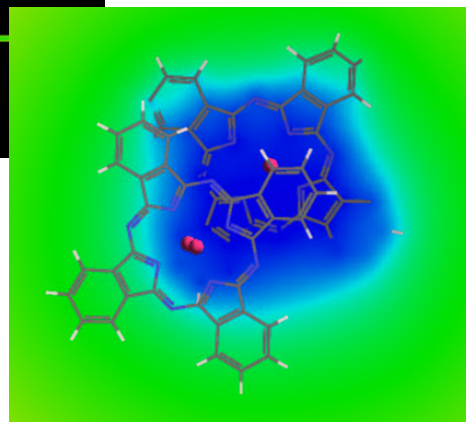


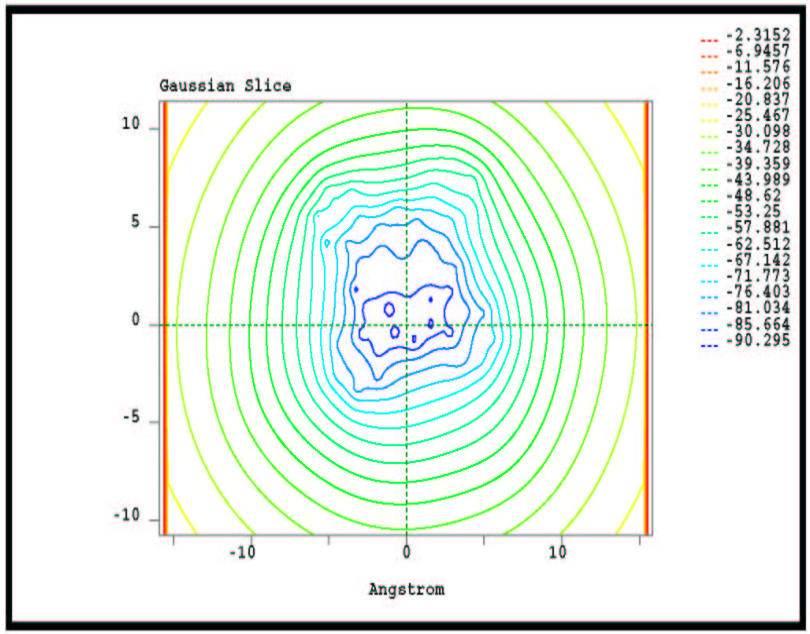
Dilithium Phthalocyanine (Li_2Pc)



Calculated Electrostatic Potential Contours Obtained from Configurations Representative of Molecular Self-assembly of Li_2Pc Molecules; Side View (Above Left), Calculated Contours are for the Li_2Pc Molecule in the Middle; Profiles of Electrostatic Potential Contours as Viewed from the Top (Right and Below) of the Molecular System

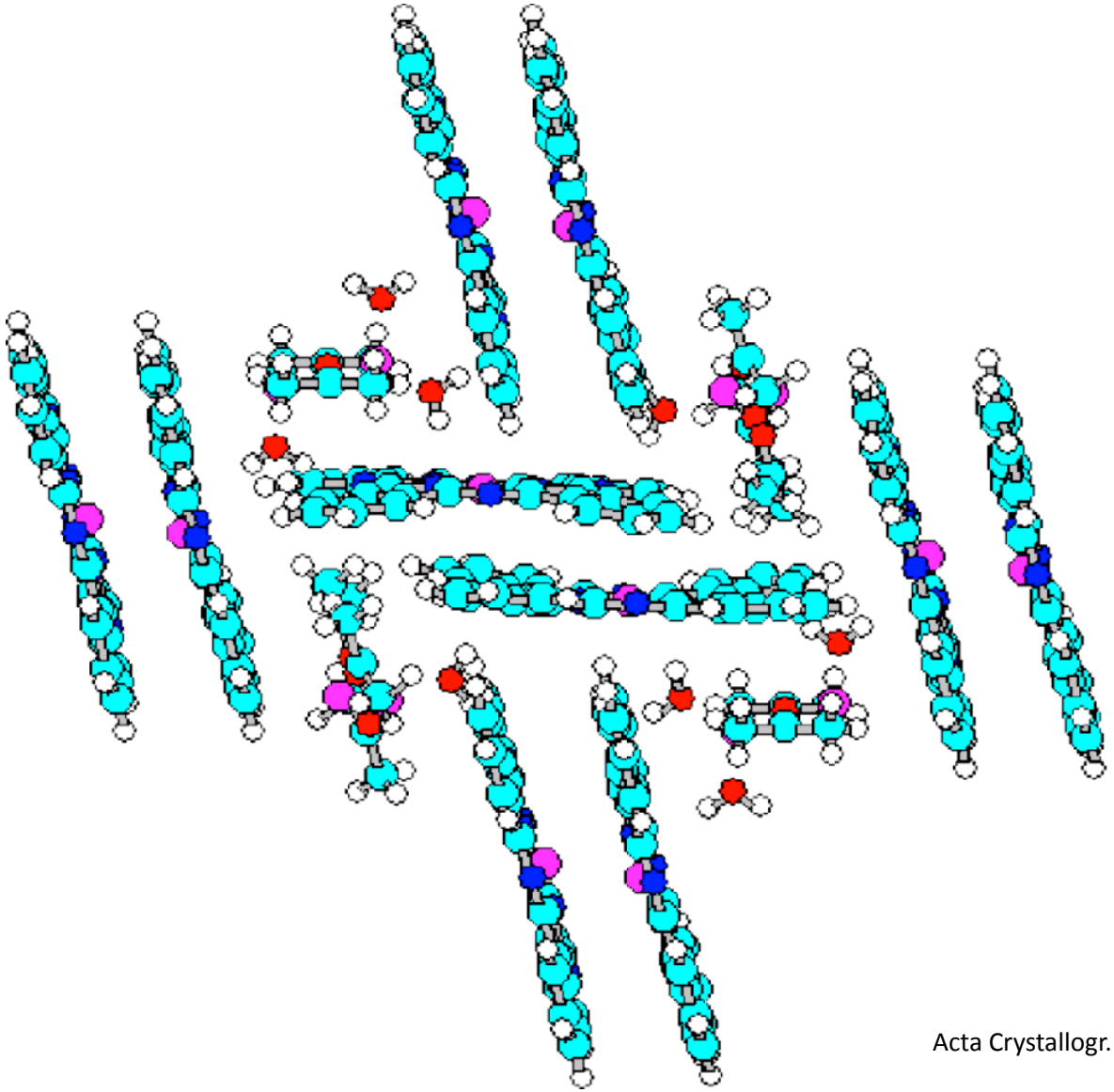






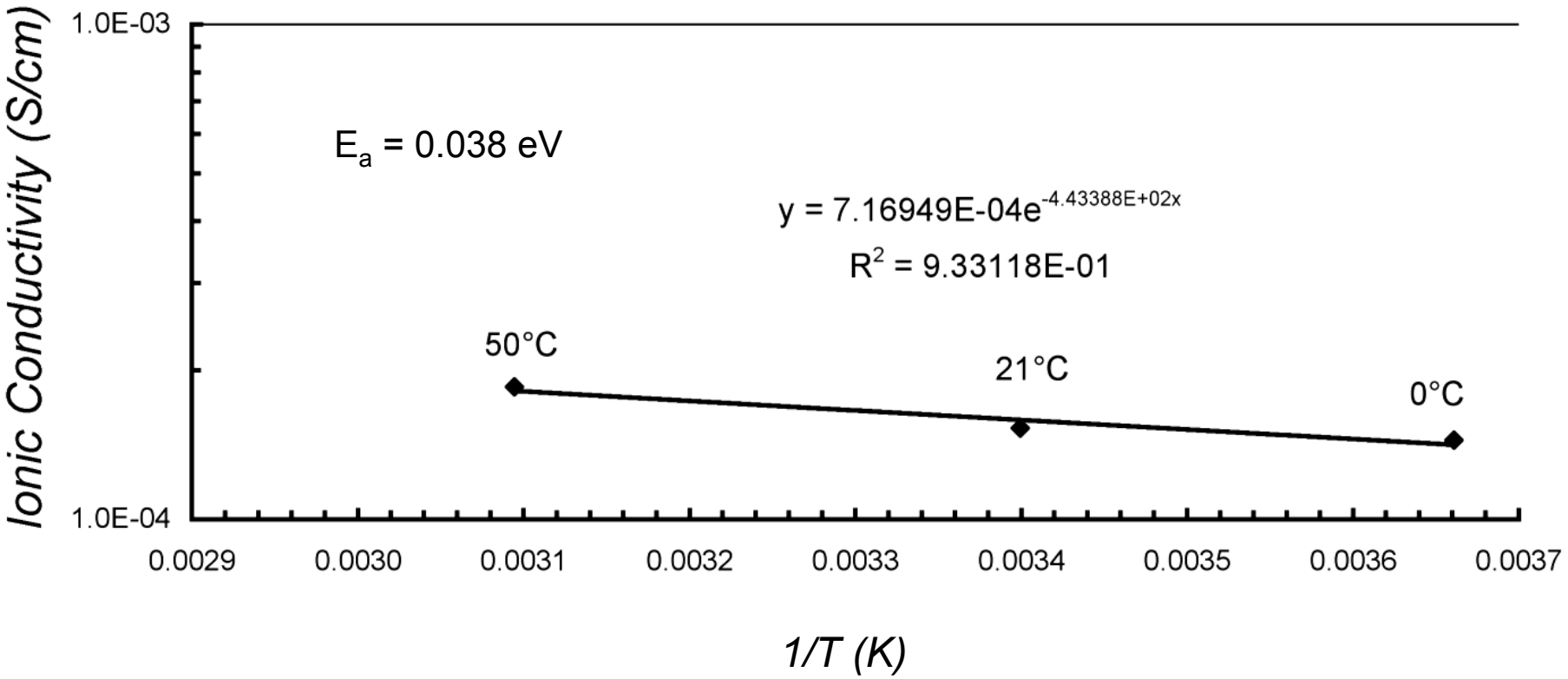
J. Phys. Chem. B, 108, 4659 (2004)

X-ray Crystal Structure of Li_2Pc



Acta Crystallogr. E62, m827-m829(2006)

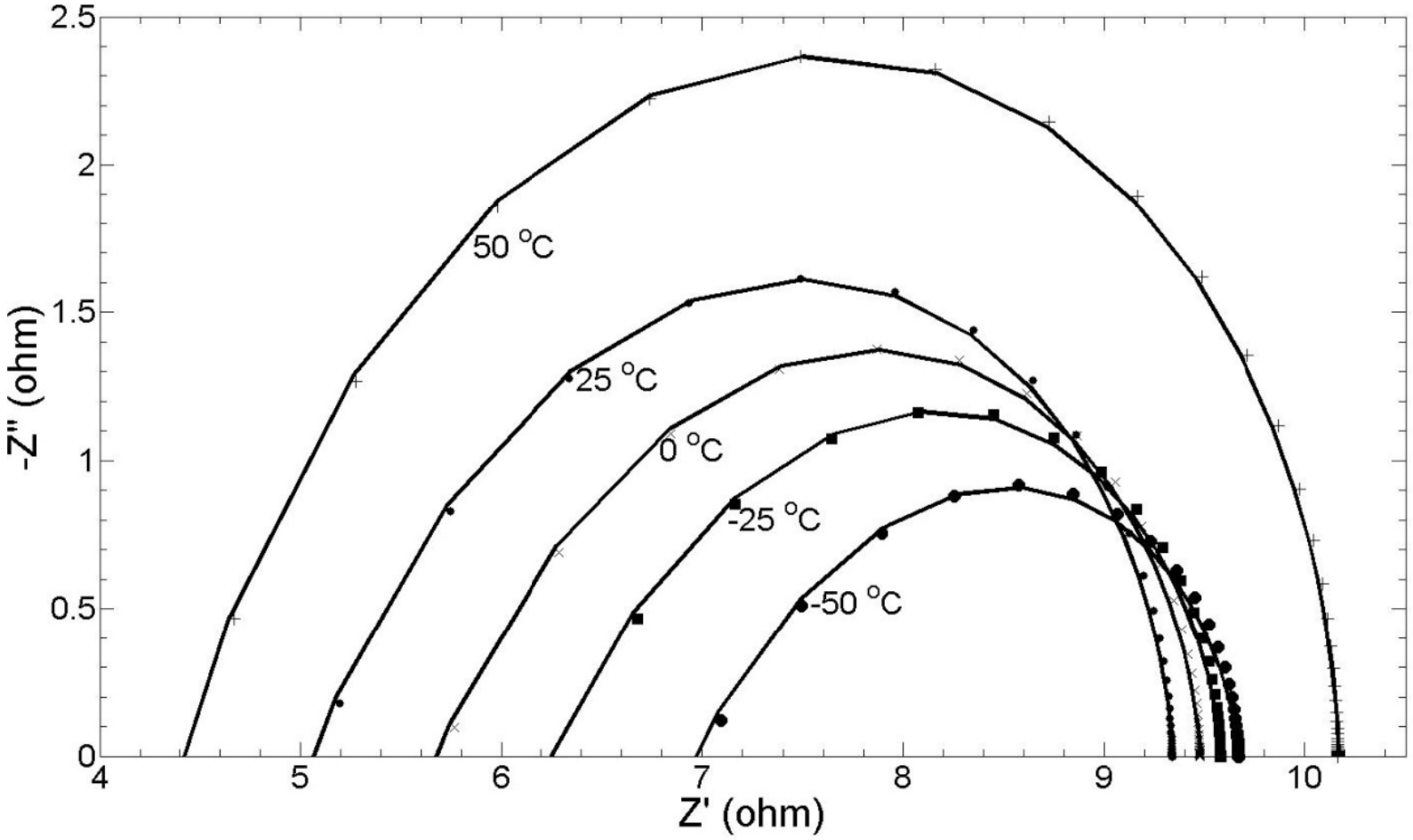
Arrhenius Plot of Ionic Conductivity for a Pressed Pellet of Single Crystals of Li_2Pc Sandwiched Between Gold Electrodes (710 µm Thick; 1.6 cm^2)



ECS Transactions, 25 (36) 163-167 (2010)

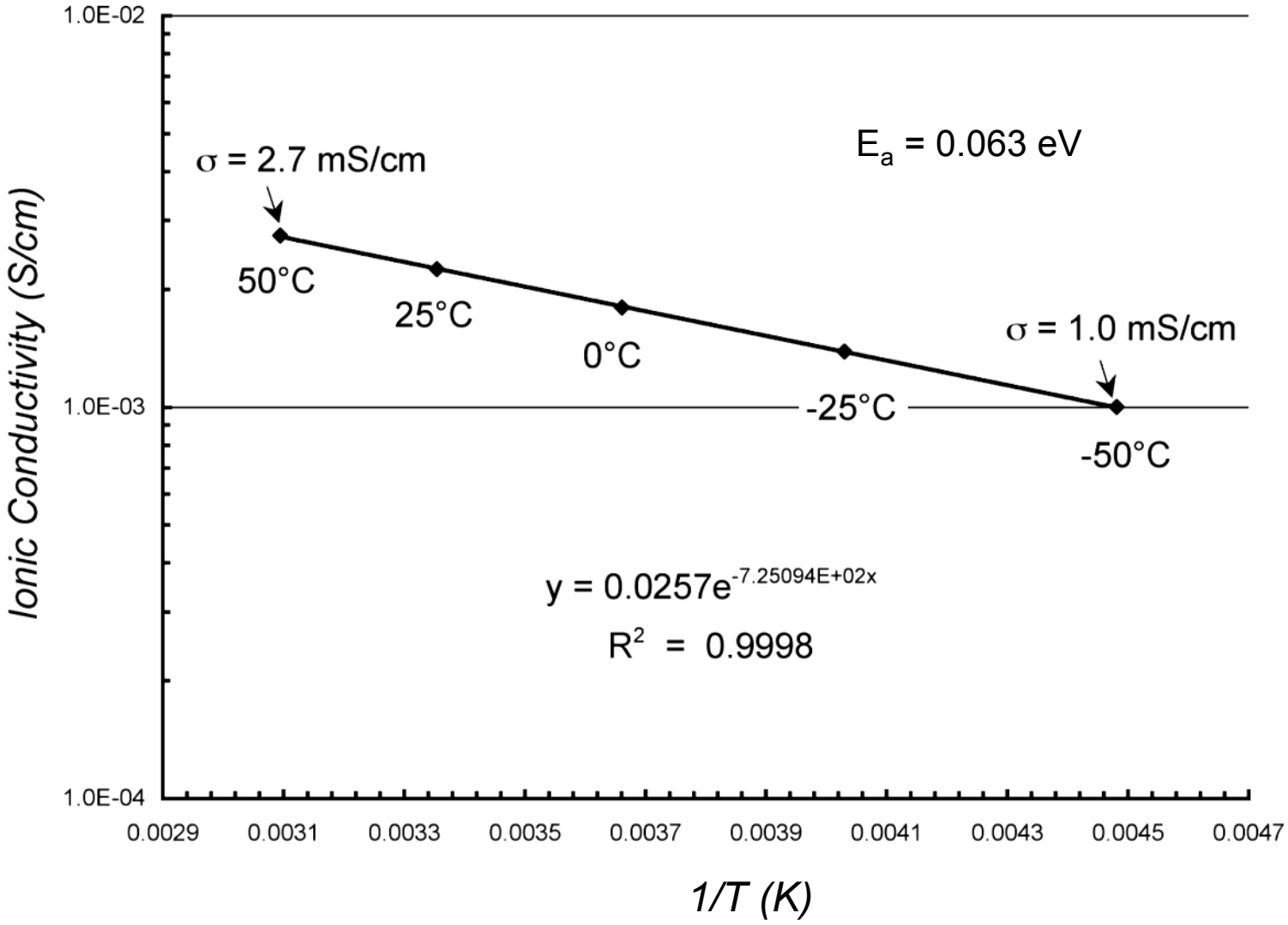
Electrochem. and Solid-State Letters, 8 (5), E45-E48 (2005)

Nyquist Plots of SS/Thin Film Li_2Pc Cast Onto an MnO_2 Cathode/SS at -50, -25, 0, +25, and 50°C



ECS Transactions, 25 (36) 163-167 (2010)

Arrhenius Plot of Ionic Conductivity for a Thin Film of Li_2Pc Cast Onto an MnO_2 Cathode at -50, -25, 0, +25, and 50°C



Conclusions

The energies of activation for ionic conduction within the pressed pellet of single crystals (0.038 eV) and the thin film of Li_2Pc dried at 160°C (0.063 eV) would suggest a very similar conduction mechanism.

The lithium ion conduction pathway might be parallel to the a-axis between the phthalocyanine rings since there is a negative electrostatic potential field between the parallel phthalocyanine rings and in effect provides a constant sphere of solvation for the lithium ion throughout the crystal lattice.

Authors

- L. G. Scanlon - Air Force Research Laboratory
- J. P. Fellner - Air Force Research Laboratory
- M. F. Lawson - Air Force Research Laboratory
- H. Xiao - Air Force Research Laboratory
- L. R. Lucente - University of Dayton Research Institute
- J. W. Lawson - University of Dayton Research Institute
- W. A. Feld - Wright State University
- P. B. Balbuena - Texas A&M University
- N. Munichandraiah - Indian Institute of Science

Acknowledgements

The authors would like to thank Dr. Chris Johnson from Argonne National Laboratory for providing the cathode for this investigation.